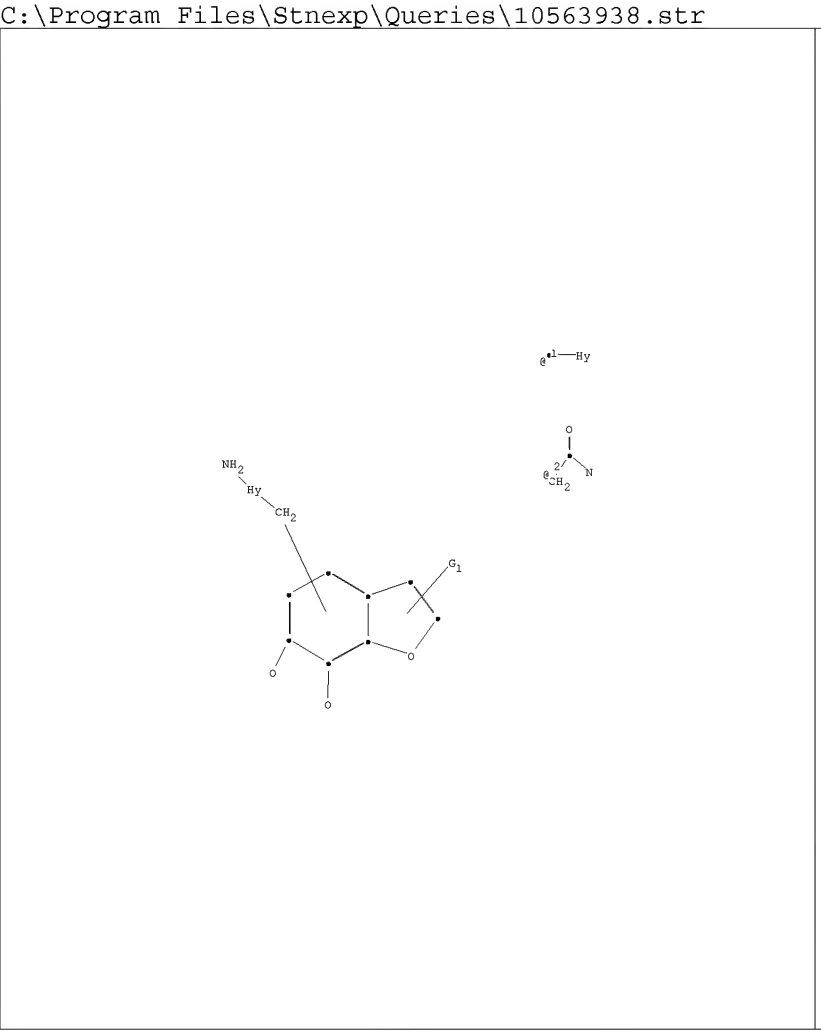
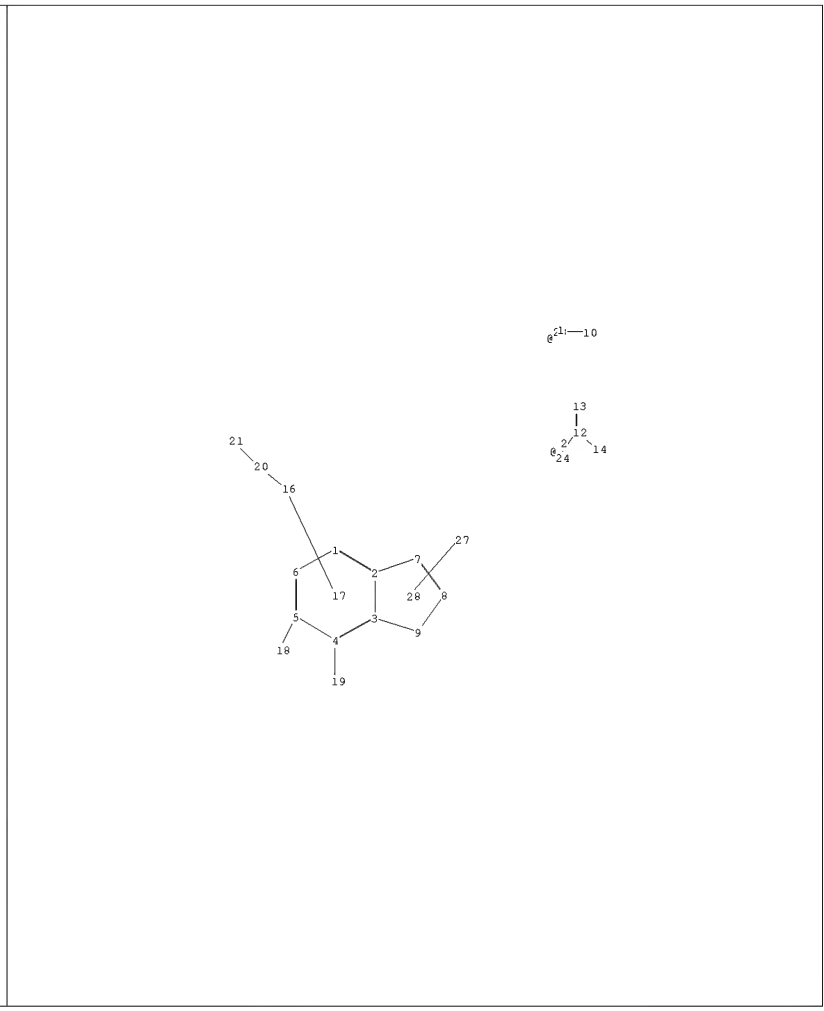
C:\Program Files\Stnexp\Queries\10563938.str





chain nodes :
    10 12 13 16 18 19 20 21 23 24 27
ring nodes :
    1 2 3 4 5 6 7 8 9
ring/chain nodes :
    14
chain bonds :
    4-19 5-18 10-23 12-13 12-14 12-24 16-20 20-21
ring bonds :
    1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9
exact/norm bonds :
    2-7 3-9 4-19 5-18 7-8 8-9 10-23 12-13 12-14 16-20 20-21
exact bonds :
    12-24
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6

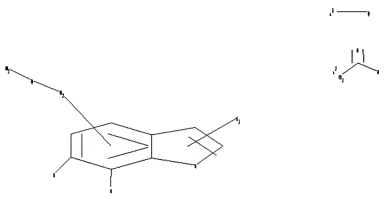
G1:CHO,[*1],[*2]

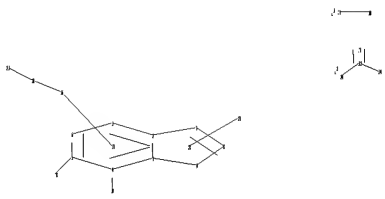
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS
    13:CLASS 14:CLASS 16:CLASS 17:Atom 18:CLASS 19:CLASS 20:Atom 21:CLASS 23:CLASS
    24:CLASS 27:CLASS 28:Atom
Generic attributes :
    10:
    Saturation   : Unsaturated
    Number of Carbon Atoms : 7 or more
    Number of Hetero Atoms : Exactly 1
    Type of Ring System   : Polycyclic
    20:
    Saturation   : Unsaturated
    Number of Carbon Atoms : less than 7
    Number of Hetero Atoms : 2 or more
    Type of Ring System   : Monocyclic

```
Element Count :
    Node 10: Limited
        C,C8
        N,N1
        O,O0
        S,S0

    Node 20: Limited
        C,C4
        N,N2
        O,O0
        S,S0
```

=>
Uploading C:\Program Files\Stnexp\Queries\10563938.str





chain nodes :
10 12 13 16 18 19 20 21 23 24 27
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
14
chain bonds :
4-19 5-18 10-23 12-13 12-14 12-24 16-20 20-21
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 8-9
exact/norm bonds :
2-7 3-9 4-19 5-18 7-8 8-9 10-23 12-13 12-14 16-20 20-21
exact bonds :

12-24
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:CHO,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:CLASS 13:CLASS 14:CLASS 16:CLASS 17:Atom 18:CLASS 19:CLASS 20:Atom
21:CLASS 23:CLASS 24:CLASS 27:CLASS 28:Atom
Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : 7 or more
Number of Hetero Atoms : Exactly 1
Type of Ring System   : Polycyclic
20:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic

Element Count :
Node 10: Limited
    C,C8
    N,N1
    O,O0
    S,S0

Node 20: Limited
    C,C4
    N,N2
    O,O0
    S,S0

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 01:40:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   7127 TO ITERATE

 28.1% PROCESSED   2000 ITERATIONS   0 ANSWERS

```
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       137479 TO   147601
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss ful
FULL SEARCH INITIATED 01:41:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   142636 TO ITERATE

100.0% PROCESSED   142636 ITERATIONS                                26 ANSWERS
SEARCH TIME: 00.00.03

L3           26 SEA SSS FUL L1

=> => s l3
L4            7 L3

=> d l4 1-7 bib,ab,hitstr
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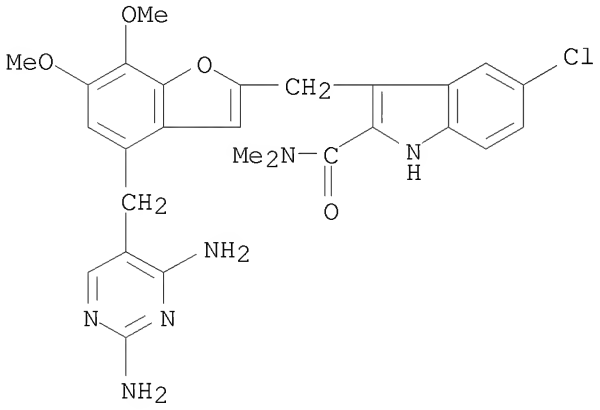
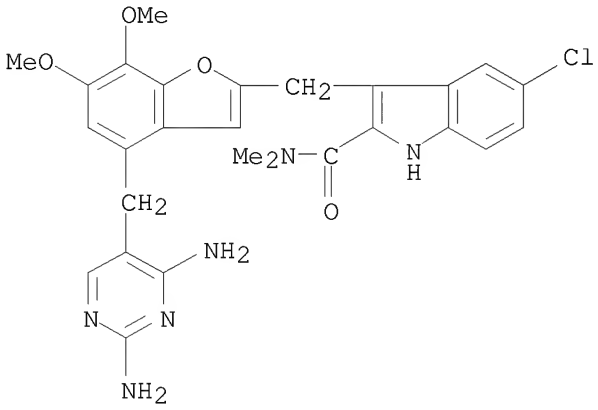
L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2008:682183 CAPLUS
TI Antistreptococcal activity of AR-709 compared to that of other agents
AU Smith, Kathy; Ednie, Lois M.; Appelbaum, Peter C.; Hawser, Stephen; Lociuro, Sergio
CS Department of Pathology, Hershey Medical Center, Hershey, PA, 17033, USA
SO Antimicrobial Agents and Chemotherapy (2008), 52(6), 2279-2282
CODEN: AMACCQ; ISSN: 0066-4804
PB American Society for Microbiology
DT Journal
LA English
AB Against 300 strains of pneumococci and 100 group A streptococci of differing β-lactam, macrolide, and quinolone resistance phenotypes, AR-709 was very active, with all MICs being ≤2 μg/mL. Furthermore, AR-709 was active against strains that were both susceptible and resistant to trimethoprim-sulfamethoxazole.
IT 663214-64-0
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(AR-709 activity against antibiotic resistant Streptococcus pneumoniae)
RN 663214-64-0 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



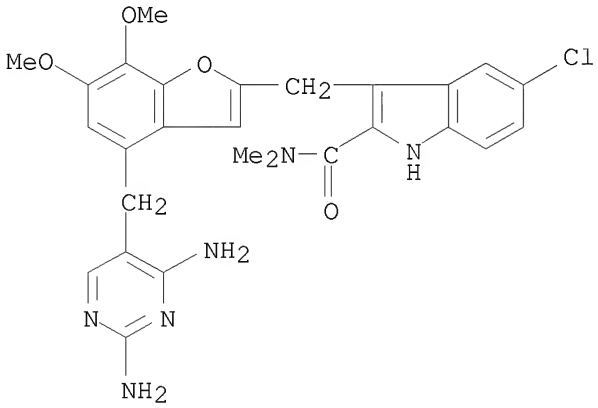
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2008:292672 CAPLUS
DN 148:280078
TI In vitro activity of AR-709 against Streptococcus pneumoniae
AU Jansen, W. T. M.; Verel, A.; Verhoef, J.; Milatovic, D.
CS University Medical Center Utrecht, Utrecht, 3584 CX, Neth.
SO Antimicrobial Agents and Chemotherapy (2008), 52(3), 1182-1183
CODEN: AMACCQ; ISSN: 0066-4804
PB American Society for Microbiology
DT Journal
LA English
AB We investigated the in vitro activity of AR-709, a novel diaminopyrimidine antibiotic currently in development for treatment of community-acquired upper and lower respiratory tract infections, against 151 Streptococcus pneumoniae strains from various European countries. AR-709 showed excellent activity against both drug-susceptible and multidrug-resistant pneumococci.
IT 663214-64-0
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(in vitro antibiotic activity of diaminopyrimidine AR-709 against Streptococcus pneumoniae)
RN 663214-64-0 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



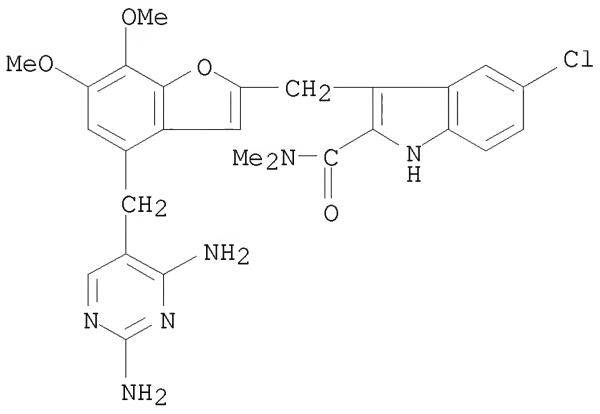
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2008:292661 CAPLUS
DN 148:280075
TI Activity of the diaminopyrimidine AR-709 against recently collected multidrug-resistant isolates of invasive Streptococcus pneumoniae from North America
AU Ressner, Roseanne A.; Moore, Matthew R.; Jorgensen, James H.
CS Brooke Army Medical Center, Fort Sam Houston, TX, USA
SO Antimicrobial Agents and Chemotherapy (2008), 52(3), 1147-1149
CODEN: AMACCQ; ISSN: 0066-4804
PB American Society for Microbiology
DT Journal
LA English
AB Broth microdilution was used to determine the MICs of AR-709 and comparator antimicrobial agents for 224 invasive multidrug-resistant isolates of Streptococcus pneumoniae. AR-709 was highly active, with a MIC50 of 0.25 μg/mL, a MIC90 of 0.5 μg/mL, and a range of ≤0.008 μg/mL to 1 μg/mL.
IT 663214-64-0, AR-709
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antibiotic activity of diaminopyrimidine AR-709 against multidrug-resistant Streptococcus pneumoniae)
RN 663214-64-0 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:901704 CAPLUS
DN 147:421821
TI Crystal Structure of the Anthrax Drug Target, Bacillus anthracis Dihydrofolate Reductase
AU Bennett, Brad C.; Xu, Hai; Simmerman, Richard F.; Lee, Richard E.; Dealwis, Chris G.
CS Department of Biochemistry, Cellular Molecular Biology, University of Tennessee, Knoxville, TN, 37996, USA
SO Journal of Medicinal Chemistry (2007), 50(18), 4374-4381
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Spores of Bacillus anthracis are the infectious agent of anthrax. Current antibiotic treatments are limited due to resistance and patient age restrictions; thus, addnl. targets for therapeutic intervention are needed. One possible candidate is dihydrofolate reductase (DHFR), a biosynthetic enzyme necessary for anthrax pathogenicity. We determined the crystal structure of DHFR from B. anthracis (baDHFR) in complex with methotrexate (MTX; 1) at 2.4 Å resolution The structure reveals the crucial interactions required for MTX binding and a putative mol. basis for how baDHFR has natural resistance to trimethoprim (TMP; 2). The structure also allows insights for designing selective baDHFR inhibitors that will have weak affinities for the human enzyme. Addnl., we have found that 5-nitro-6-methylamino-isocytosine (MANIC; 3), which inhibits another B. anthracis folate synthesis enzyme, dihydropteroate synthase (DHPS), can also inhibit baDHFR. This provides a starting point for designing multi-target inhibitors that are less likely to induce drug resistance.
IT 663214-64-0D, AR 709, complexes with dihydrofolate reductase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(crystal structure of Bacillus anthracis dihydrofolate reductase)
RN 663214-64-0 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD

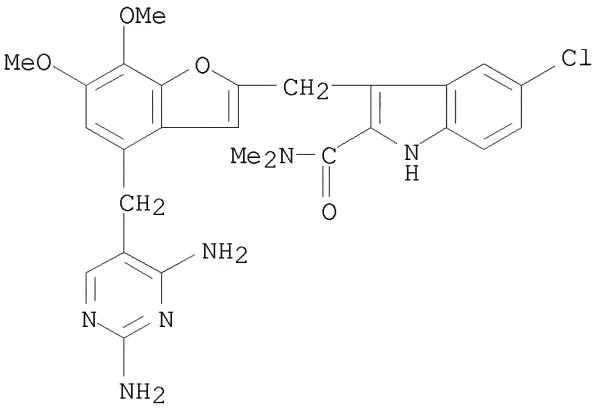
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:847673 CAPLUS
DN 145:249225
TI Novel process for the preparation of 5-chloro-3-[4-(2,4-diaminopyrimidin-5-ylmethyl)-6,7-dimethoxybenzofuran-2-ylmethyl]-1H-indole-2-carboxylic acid dimethylamide
IN Schneider, Peter; Tahtaoui, Chouaib; Braun, Martin; Greiveldinger-Poenaru, Sorana; Jaeger, Juergen; Schmitt, Laurent
PA Arpida AG, Switz.
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006087140	A1	20060824	WO 2006-EP1179	20060210
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	AU 2006215785	A1	20060824	AU 2006-215785	20060210
	CA 2596668	A1	20060824	CA 2006-2596668	20060210
	EP 1856109	A1	20071121	EP 2006-706809	20060210
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
	EE 200700050	A	20071217	EE 2007-50	20060210
	HU 2007000605	A2	20080128	HU 2007-605	20060210
	HU 2007000605	A3	20080228		
	NO 2007003678	A	20070903	NO 2007-3678	20070717
	MX 200709283	A	20080219	MX 2007-9283	20070801
	CN 101115746	A	20080130	CN 2006-80003963	20070803
	KR 2007106636	A	20071102	KR 2007-721395	20070918
PRAI	WO 2005-EP1695	A	20050218		
	EP 2005-1695	A	20050218		
	WO 2006-EP1179	W	20060210		

OS CASREACT 145:249225; MARPAT 145:249225
AB The invention relates to a novel process for the preparation of [[(pyrimidinylmethyl)benzofuranyl]methyl]indolecarboxamide derivative I, a dihydrofolate reductase inhibitor with antibiotic properties. Starting compds. for the synthesis are 5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-pyrimidinediamine (trimethoprim) and 5-chloro-1H-indole-2-carboxylic acid dimethylamide and the key intermediates are II (R = t-Bu, i-Pr).
IT 663214-64-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(Novell processes for the preparation of a benzofuran)
RN 663214-64-0 CAPLUS

CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



IT 905928-48-5P 905928-53-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Novell processes for the preparation of a benzofuran)

RN 905928-48-5 CAPLUS

CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]carbonyl]-N,N-dimethyl-, methanesulfonate (1:1) (CA INDEX NAME)

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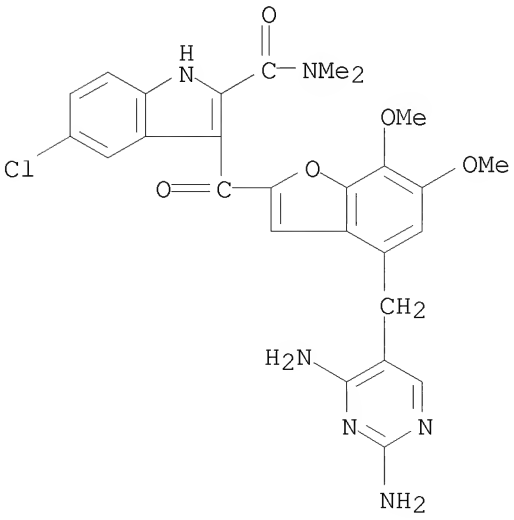
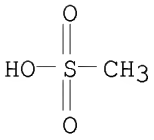
CRN 905928-47-4
CMF C27 H25 Cl N6 O5

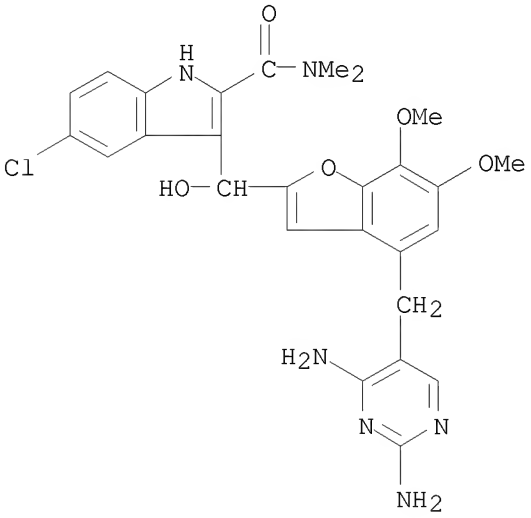


CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 905928-53-2 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]hydroxymethyl]-N,N-dimethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:227939 CAPLUS
DN 144:274296
TI Preparation of pyrimidinylmethyl substituted benzofuran derivatives and their use in the treatment of microbial infections
IN Greiveldinger-Poenaru, Sorana; Islam, Khalid; Gillessen, Dieter; Burri, Kaspar
PA Arpida AG, Switz.
SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DT Patent
LA English

Applicant's

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005005418	A1	20050120	WO 2004-EP7482	20040708
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004255344	A1	20050120	AU 2004-255344	20040708
	CA 2531757	A1	20050120	CA 2004-2531757	20040708
	EP 1651639	A1	20060503	EP 2004-763125	20040708
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	CN 1820004	A	20060816	CN 2004-80019414	20040708
	BR 2004012425	A	20060905	BR 2004-12425	20040708
	HU 2006000114	A2	20070928	HU 2006-114	20040708
	MX 2005PA14081	A	20060309	MX 2005-PA14081	20051220
	NO 2005006254	A	20060208	NO 2005-6254	20051230
	IN 2006CN00081	A	20070629	IN 2006-CN81	20060106
	US 20060154943	A1	20060713	US 2006-563938	20060110
PRAI	WO 2003-EP7537	A	20030711		
	WO 2004-EP7482	W	20040708		

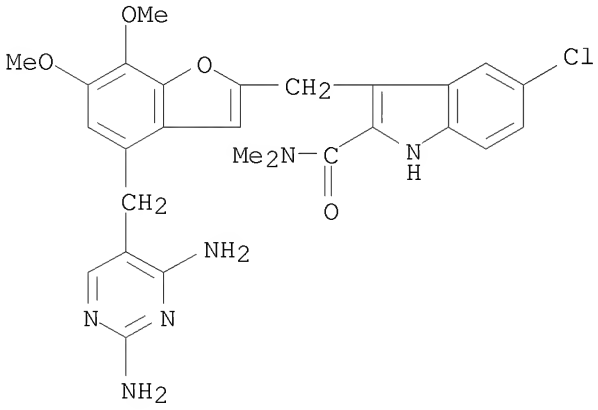
OS CASREACT 144:274296; MARPAT 144:274296

AB The invention relates to new title compds. I [R1 = II (wherein R5 = H, alkyl, C(O)NR8R9; R8 = alkoxy, alkylamino, alkyl; R9 = alkyl; NR8R9 = 5-6 membered heterocyclic ring containing 1-2 heteroatoms which can be the same or different and are O or N; R6 = H, halo, NO2, alkoxy; R7 = H); R2, R3 = H, alkyl; or R2 and R3 together represent alkylene with 1-3 carbon atoms bridging the oxygen atoms and forming a 5-7 membered ring; R4 = H] which are useful for treating infections caused by Gram pos. or Gram neg. pathogens. Preparation of compds. I is described in 21 synthetic examples. Thus, reacting 5-(2-chloromethyl-6,7-dimethoxybenzofuran-4-ylmethyl)pyrimidine-2,4-diamine with indole afforded 23% 5-[2-(1H-indol-3-ylmethyl)-6,7-dimethoxybenzofuran-4-ylmethyl]pyrimidine-2,4-diamine. It has been found that compds. I are more potent than, e.g., Trimethoprim, and are active against Gram pos. pathogens and Gram neg. pathogens. Furthermore, I show a much more potent activity against DHFR including mutated enzyme, a superior bioavailability, and a superior

antibacterial activity. Thus, the minimal inhibition concentration (MIC) of the compds. I regarding resistant strains is in the range of 0.25-2.0 μg/mL depending on the strain used. The IC50 of the compds. I regarding DHFR mutants is in the range of 0.5-8.0 μM. The invention also concerns related aspects including processes for the preparation of the compds. I, pharmaceutical compns. containing one or more of those compds. and especially their use as anti-infectives.

IT 663214-64-0P 878156-91-3P 878156-92-4P
878156-93-5P 878156-94-6P 878156-95-7P
878156-96-8P 878156-97-9P 878156-98-0P
878156-99-1P 878157-00-7P 878157-01-8P
878157-02-9P 878157-03-0P 878157-04-1P
878157-05-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinylmethyl substituted benzofuran derivs. for treating microbial infections)

RN 663214-64-0 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



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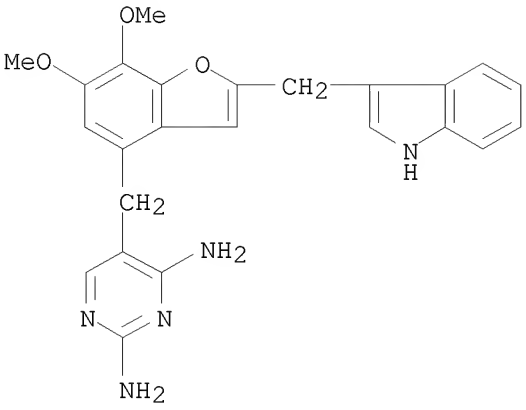
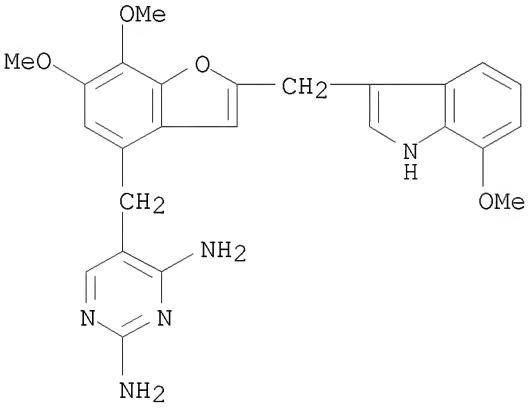
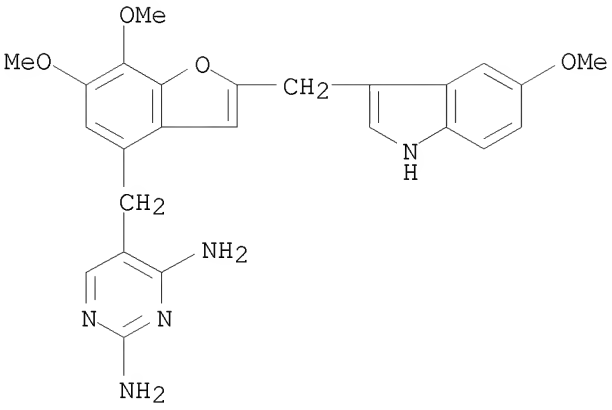
CN 2,4-Pyrimidinediamine, 5-[[2-(1H-indol-3-ylmethyl)-6,7-dimethoxy-4-benzofuranyl]methyl]- (CA INDEX NAME)



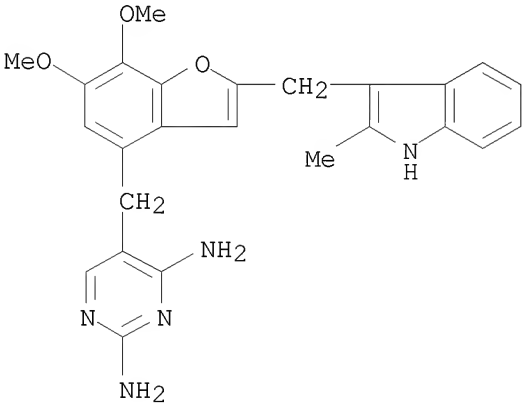
RN 878156-92-4 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[6,7-dimethoxy-2-[(7-methoxy-1H-indol-3-yl)methyl]-4-benzofuranyl]methyl]- (CA INDEX NAME)



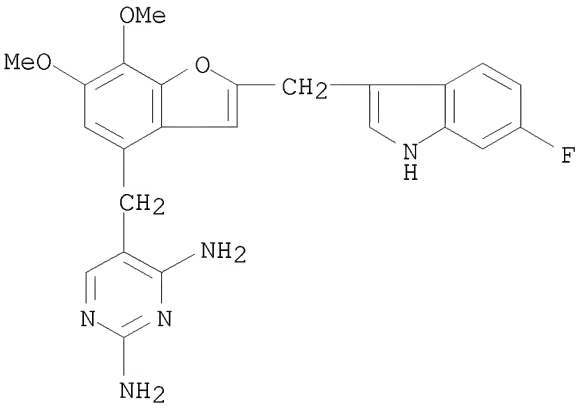
RN 878156-93-5 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[6,7-dimethoxy-2-[(5-methoxy-1H-indol-3-yl)methyl]-4-benzofuranyl]methyl]- (CA INDEX NAME)



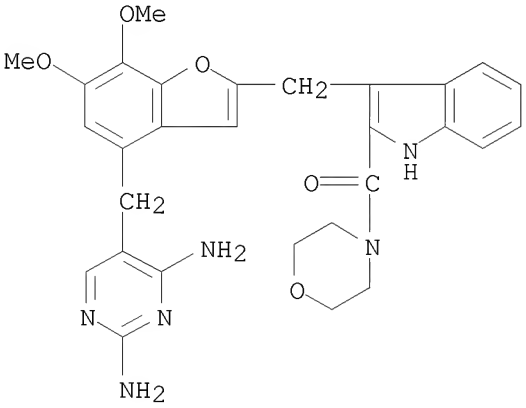
RN 878156-94-6 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[6,7-dimethoxy-2-[(2-methyl-1H-indol-3-yl)methyl]-4-benzofuranyl]methyl]- (CA INDEX NAME)



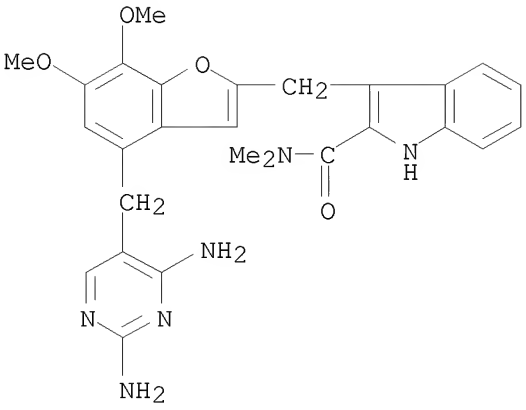
RN 878156-95-7 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[2-[(6-fluoro-1H-indol-3-yl)methyl]-6,7-dimethoxy-4-benzofuranyl]methyl]- (CA INDEX NAME)



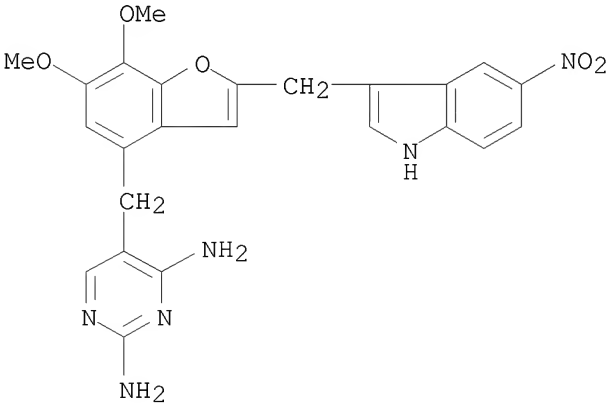
RN 878156-96-8 CAPLUS
CN Methanone, [3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-1H-indol-2-yl]-4-morpholinyl- (CA INDEX NAME)



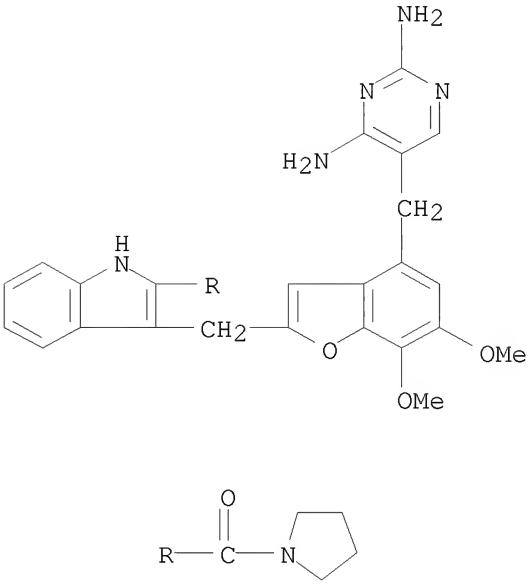
RN 878156-97-9 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N,N-dimethyl- (CA INDEX NAME)



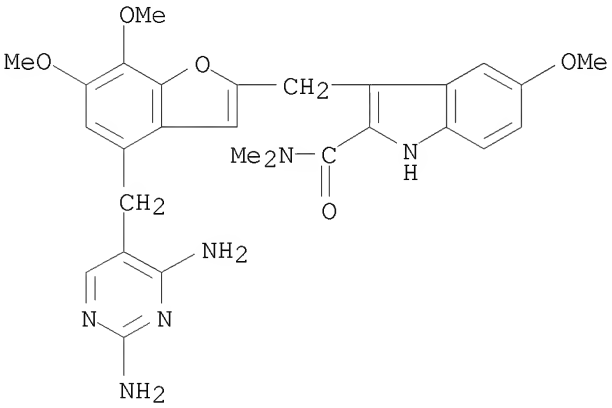
RN 878156-98-0 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[6,7-dimethoxy-2-[(5-nitro-1H-indol-3-yl)methyl]-4-benzofuranyl]methyl]- (CA INDEX NAME)



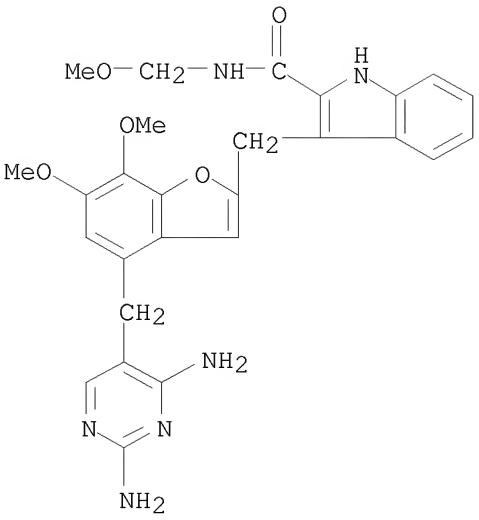
RN 878156-99-1 CAPLUS
CN Methanone, [3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-1H-indol-2-yl]-1-pyrrolidinyl- (CA INDEX NAME)



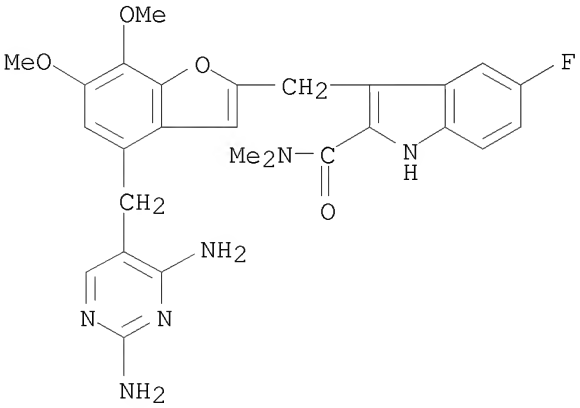
RN 878157-00-7 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-5-methoxy-N,N-dimethyl- (CA INDEX NAME)



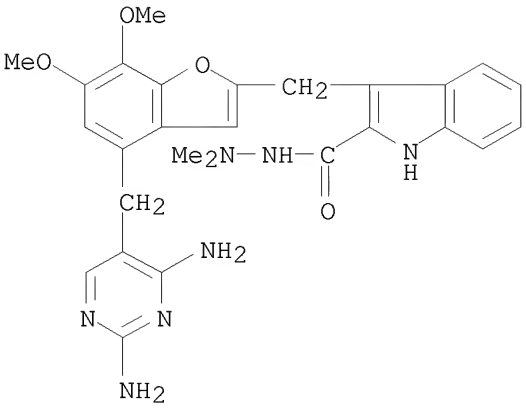
RN 878157-01-8 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N-(methoxymethyl)- (CA INDEX NAME)



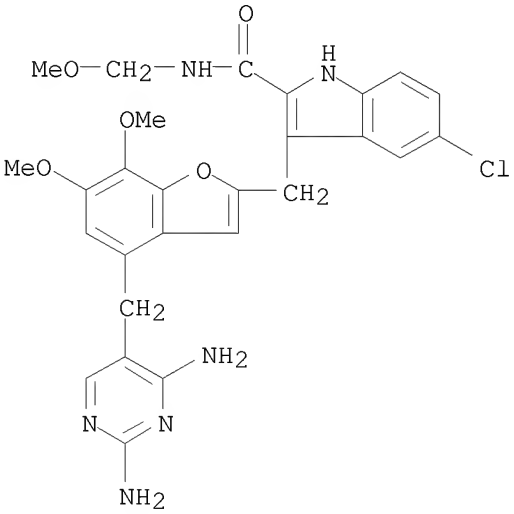
RN 878157-02-9 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-5-fluoro-N,N-dimethyl- (CA INDEX NAME)



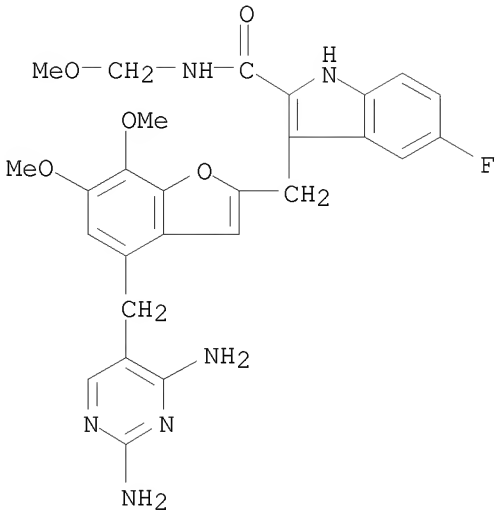
RN 878157-03-0 CAPLUS
CN 1H-Indole-2-carboxylic acid, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-, 2,2-dimethylhydrazide (CA INDEX NAME)



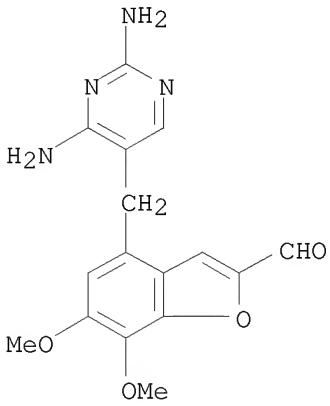
RN 878157-04-1 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-N-(methoxymethyl)- (CA INDEX NAME)



RN 878157-05-2 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[[4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy-2-benzofuranyl]methyl]-5-fluoro-N-(methoxymethyl)- (CA INDEX NAME)



IT 878157-09-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinylmethyl substituted benzofuran derivs. for treating microbial infections)
RN 878157-09-6 CAPLUS
CN 2-Benzofurancarboxaldehyde, 4-[(2,4-diamino-5-pyrimidinyl)methyl]-6,7-dimethoxy- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:107337 CAPLUS
DN 136:151176
TI Benzofuran-containing 2,4-diamino-5-substituted-pyrimidine derivatives and their preparation and use as antibacterial agents
IN Burri, Kaspar; Greiveldinger-Poenaru, Sorana; Islam, Khalid
PA Arpida A.-G., Switz.
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002010156	A1	20020207	WO 2000-EP7357	20000729
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2417401	A1	20020207	CA 2001-2417401	20010720
	WO 2002010157	A1	20020207	WO 2001-EP8426	20010720
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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	EP 1307445	A1	20030507	EP 2001-969459	20010720
	EP 1307445	B1	20051221		
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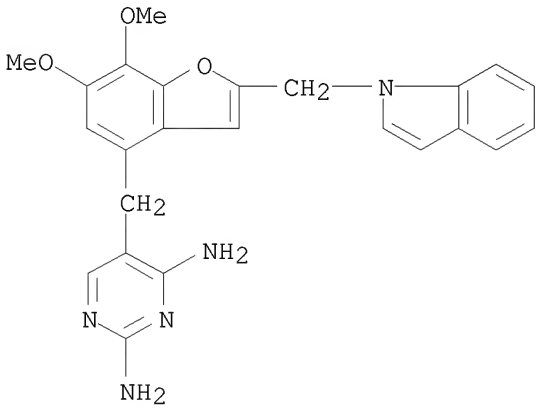
	JP 2004505077	T	20040219	JP 2002-515886	20010720
	AT 313541	T	20060115	AT 2001-969459	20010720
	ES 2250474	T3	20060416	ES 2001-969459	20010720
	TW 283674	B	20070711	TW 2001-90119335	20010808
	MX 2003PA00606	A	20040402	MX 2003-PA606	20030121
	US 20040034047	A1	20040219	US 2003-333853	20030123
	US 7030130	B2	20060418		
	NO 2003000417	A	20030127	NO 2003-417	20030127
PRAI	WO 2000-EP7357	A	20000729		
	WO 2001-EP8426	W	20010720		

OS MARPAT 136:151176
AB The invention relates to novel benzofuran derivs. I and their use as active ingredients in the preparation of pharmaceutical compns. [wherein: R1 = alkyl, cycloalkylmethyl, alkylcarbonyl, cycloalkylcarbonyl, cycloalkylhydroxymethyl, alkenyl, (un)substituted (hetero)arylmethyl, arylcarbonyl, or arylhydroxymethyl; R2, R3 = H, alkyl; or R2R3 = C1-3 alkylene giving 5- to 7-membered ring; R4 = H, alkyl; including pharmaceutically acceptable salts and N-oxides]. The invention also concerns related aspects, including processes for the preparation of the compds., pharmaceutical compns. containing one or more of them, and especially their use as anti-infectives. Claims include 36 specific compds., and the syntheses of 3 especially preferred compds. are described. For instance, Me 3,4,5-trimethoxybenzoate underwent 2-formylation, 3-O-demethylation, cyclocondensation with 2-bromo-1-cyclopropylethanone, and reduction of the

ketone with TMS-Cl and NaBH3CN, to give 6,7-dimethoxy-2-cyclopropylmethylbenzofuran-4-carboxylic acid Me ester. The latter ester underwent reduction to the 4-aldehyde using Red-Al, followed by condensation with 3-anilinopropionitrile, and cyclocondensation of the resulting anilinoacrylonitrile derivative with guanidine HCl, to give highly preferred title compound II. Compds. I are more potent than, e.g., trimethoprim (no data). They are especially active against both gram-pos. and gram-neg. pathogens, and are especially potent against respiratory tract pathogens.

IT 394736-11-9P, 5-[[6,7-Dimethoxy-2-(indol-1-ylmethyl)benzofuran-4-yl]methyl]pyrimidine-2,4-diamine 394736-17-5P, 5-[[6,7-Dimethoxy-2-(indol-1-ylcarbonyl)benzofuran-4-yl]methyl]pyrimidine-2,4-diamine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzofuran-containing diaminopyrimidine derivs. as antibacterial agents)

RN 394736-11-9 CAPLUS
CN 2,4-Pyrimidinediamine, 5-[[2-(1H-indol-1-ylmethyl)-6,7-dimethoxy-4-benzofuranyl]methyl]- (CA INDEX NAME)



RN 394736-17-5 CAPLUS
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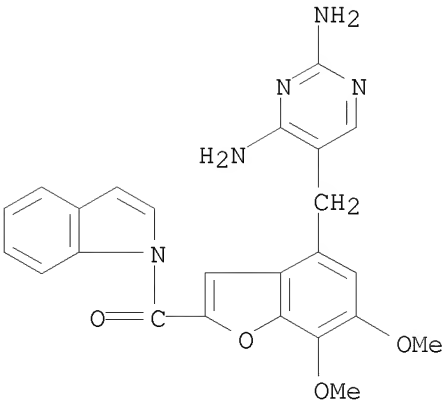

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    38.63     217.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -5.60      -5.60

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